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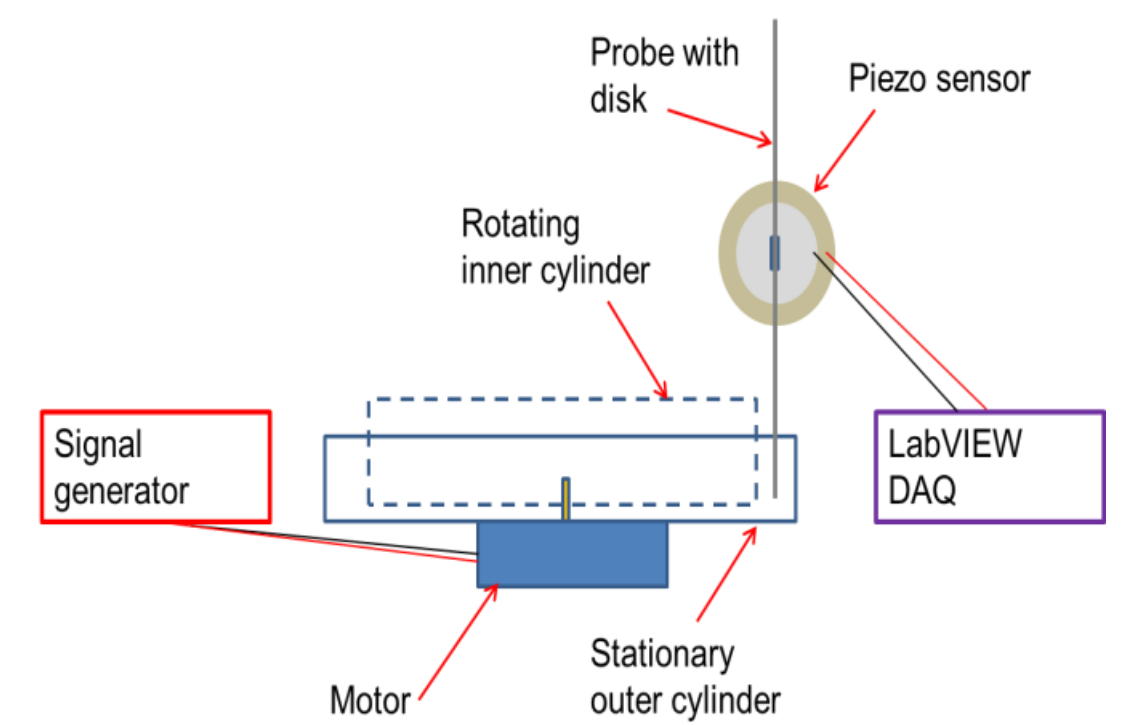
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Summary

- Jamming occurs in a multitude of different systems on various length and time scales.
- Underlying mechanisms are not clearly understood.
- Can simulations verify behaviour and patterns found in experiments?
- Can manipulation of thermostats mimic the hydrodynamic interactions?

Experimental Method

- Couette system with densely packed colloidal particles.
- Intermittent jamming detected by needle and piezo sensor inserted in system.
- Magnitude of jamming event related to voltage



Equations of Motion

$$\dot{\mathbf{r}}_i = \frac{\mathbf{p}_i}{m} + \dot{\gamma} y_i \mathbf{e}_x + \frac{s}{T} \frac{\partial T_{conf}}{\partial \mathbf{r}_i}$$

$$\dot{\mathbf{p}}_i = \mathbf{F}_i - \dot{\gamma} p_{yi} \mathbf{e}_x - \alpha \mathbf{p}_i$$

$$\dot{s} = -Q \frac{(T_{conf} - T)}{T}$$

Kinetic

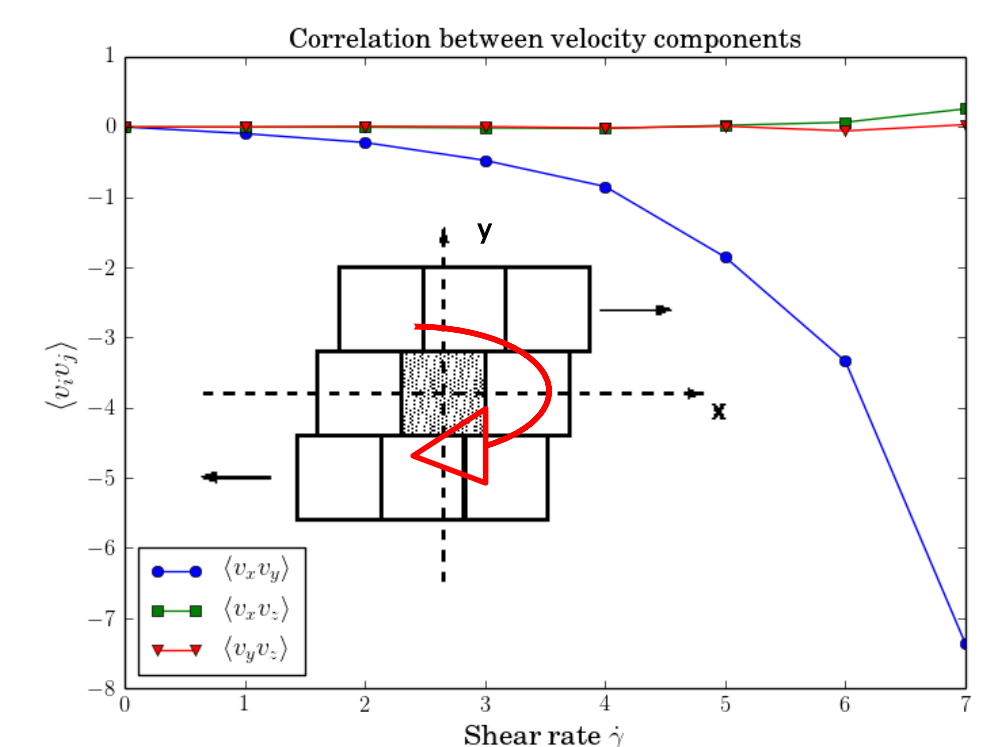
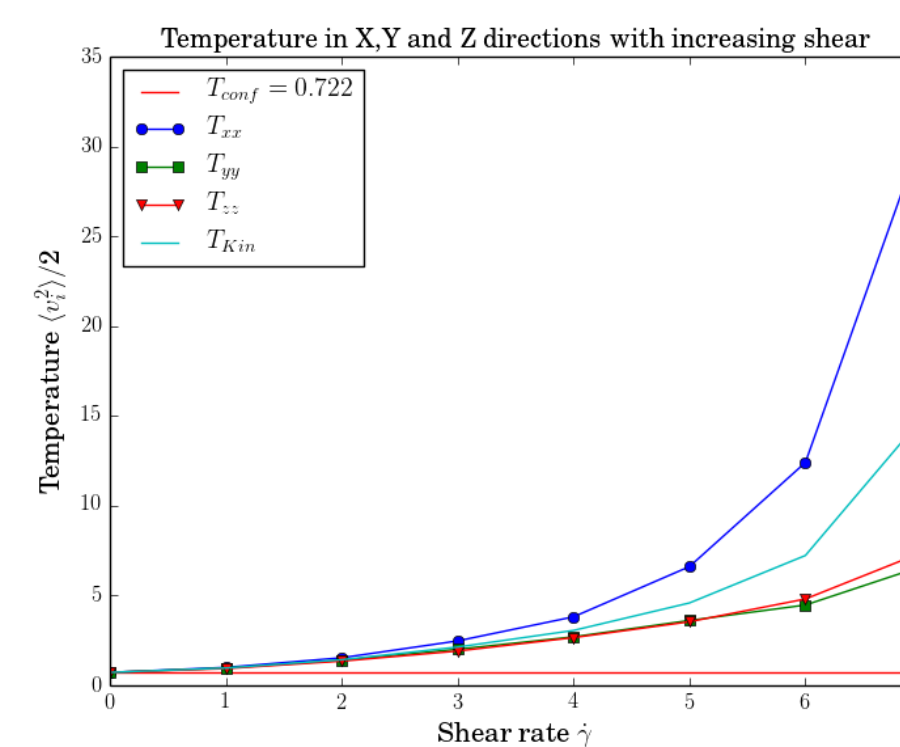
Configurational

$$\sum_i \left\langle \frac{mv_i^2}{2} \right\rangle = \frac{3}{2} k T_{kin} \quad \frac{1}{k_B T_{conf}} = \left\langle \frac{\sum_i \frac{\partial^2 \Phi_0}{\partial \mathbf{r}_i^2}}{\sum_i \left(\frac{\partial \Phi_0}{\partial \mathbf{r}_i} \right)^2} \right\rangle$$

- Kinetic temperature defined by velocities, configurational defined by positions.

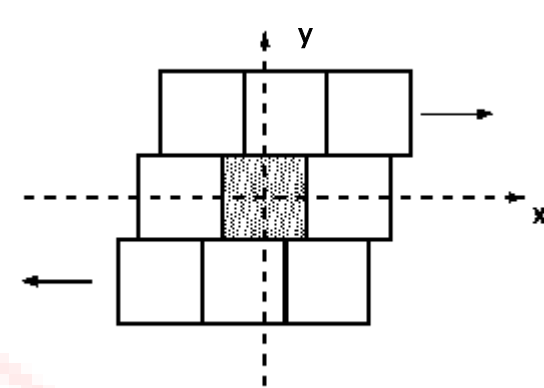
Shear Thickening with CT Thermostat

- Use of configurational thermostat leads to shear thickening regimes for this system.
- Kinetic degrees of freedom allowed to fluctuate – no lane formation observed.
- Kinetic temperature differs in X, Y and Z directions.
- Strong correlation between X and Y velocity components (Reynolds stress).



Simulation Methods

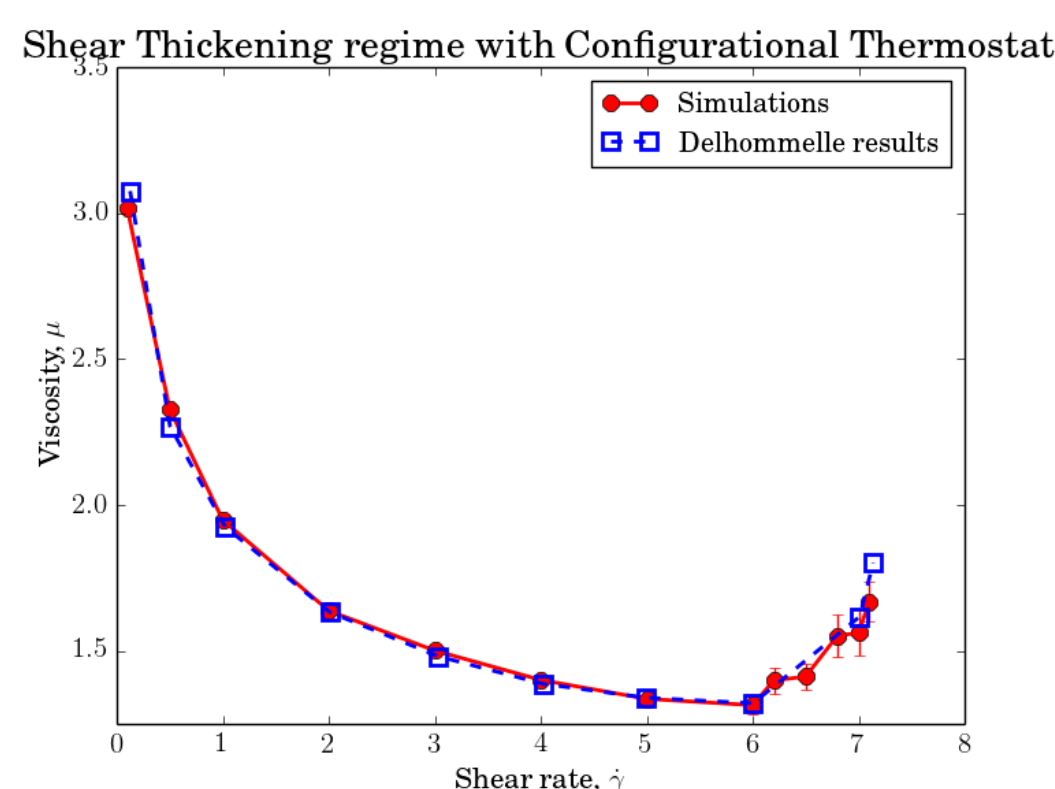
- Numerical Integration with 4th order Gear predictor–corrector algorithm.
- Lees Edwards boundary conditions (sliding brick)



Benchmarking code

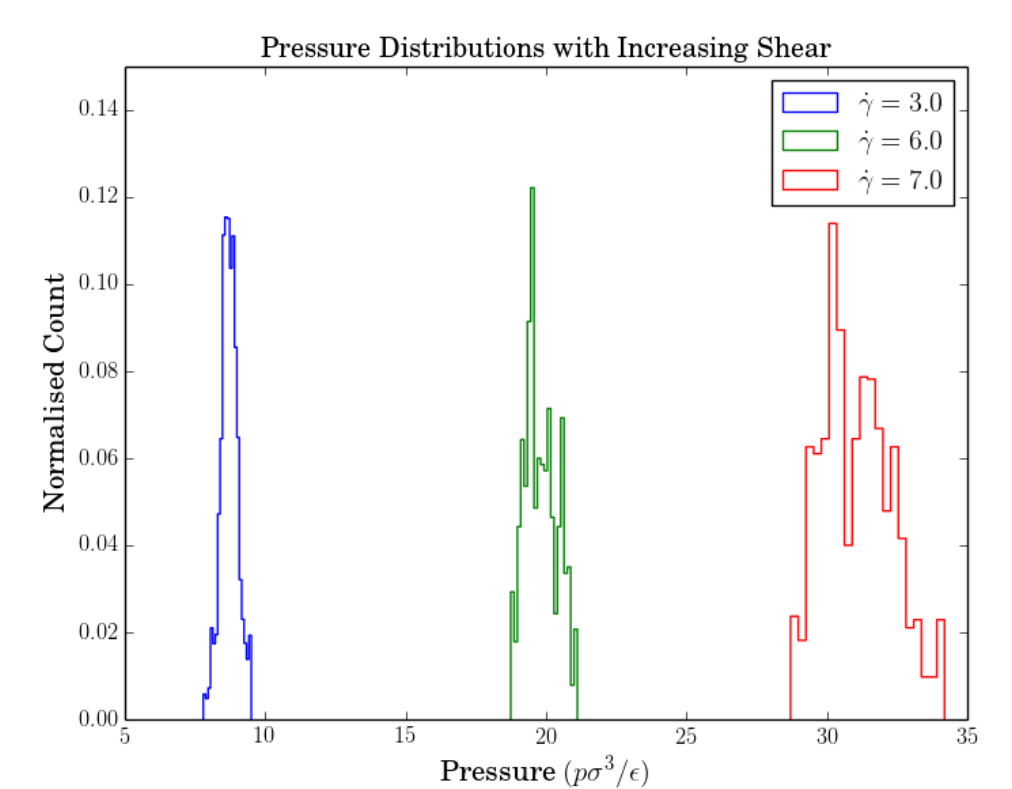
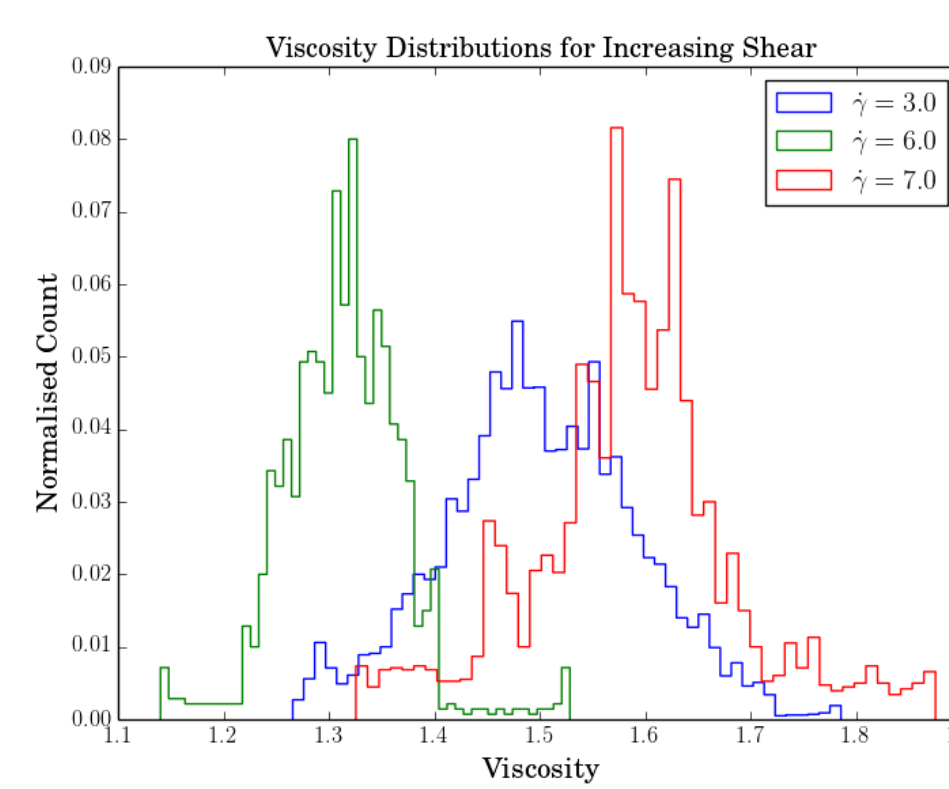
Comparison of shear thickening regime with configurational thermostat [1].

- $T_{conf} = 0.722$
- $n = N/V = 0.844$
- $N = 1372$ particles
- L-J potential



System Properties

- Histograms of fluctuations in viscosity at particular shear rates obtained.
- Similarly, pressure distributions were also obtained.
- Evident broadening of distribution occurring at highest shear rates, indicating larger fluctuations in stresses during shear thickening.



Conclusions

- Shear thickening regime obtained using configurational thermostat.
- By thermostating configurationally; velocities are allowed to freely deviate from streamline, giving insight to Reynolds stress.
- Currently parallelising code to simulate larger systems and obtain longer trajectories for better statistics in shear thickening regime.